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# Application of PestLCI model to site-specific soil and climate conditions: the case of maize production in Northern Italy

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## Abstract

*The calculation of emissions from the use of pesticides is a critical issue in LCA studies of agri-food products and only occasionally discussed in details in literature studies. The objective of this study is to assess the results of the application of PestLCI 2.0 model to the production of maize in Northern Italy using site-specific soil and climate data, which were added for this purpose in PestLCI database. In this way, the application of the tool and its database were tailored to that area. Moreover, the results were compared with those obtained assuming maize cultivation on other soil typologies in the surrounding areas. Results show that soil variation scarcely affects the emissions to air and surface water whereas it affects significantly the emissions to groundwater. Finally, some features of PestLCI were highlighted and comments for a further improvement of the model were provided.*

## 1. Introduction

The calculation of on-field emissions from the use of pesticides is often a critical issue in LCA studies of agri-food production chains, because of the following reasons: I) lack of knowledge about toxicological properties of chemicals (European Commission, 2001); II) the complexities involved in toxicity effect modelling (IEA Bioenergy, 2015); III) lack of scientific consensus on which model should be adopted for the calculation of emissions into air, soil and water; IV) lack of completeness on how pesticides are inventoried and characterized in the impact assessment phase (Garavini et al., 2015). All these issues explain why the toxicity impacts due to pesticide applications are often omitted from LCA studies or not discussed in detail. According to Notarnicola et al. (2015), there are two main approaches for estimating pesticides emissions: I) the estimation of emissions to air, groundwater and surface water, by means of models such as Margni et al. (2002) and PestLCI 2.0 (Dijkman et al., 2012); II) the assumption that all pesticides applied end up as emissions to soil (Nemecek and Kagi, 2007).

In particular, PestLCI 2.0 is a detailed model in which a pesticide is considered as an emission when it crosses the boundary between the technosphere and ecosphere that is defined by the technosphere box. This technosphere box consists of the field, including the soil up to 1 m depth and the air column up to 100 m above the field. Within the technosphere box, a number of primary and secondary processes determine the fate of the pesticide. Primary processes occur directly after pesticide application: a part of the applied pesticide drifts away from the field, the remaining part is distributed over the crops in the field and the field soil. Secondary processes then determine the fate of the pesticide present in the field. The fraction of pesticide deposited on crop is subject to degradation, uptake into the plant tissues, and volatilization (emission to air). In the top soil, degradation and volatilization (emission to air) are modelled. At the first rainfall event after pesticide application, the pesticide remaining on the leaves are assumed to wash off to soil. Together with the pesticide remaining on the top soil, this fraction is susceptible for runoff (emission to surface water) and macropore flow (emission to ground water). The remaining fraction of pesticide is assumed to enter the subsoil where it starts leaching through the soil matrix. In the subsoil, pesticide can be degraded, intercepted by drainage tubes (emission to surface water) or become an emission to groundwater, which is the case once the pesticide reaches 1 m depth.

PestLCI 2.0 was developed for modelling European conditions, but local circumstances may not be reflected in the modelling. For example, runoff of dissolved pesticide is reported as an emission to surface water, thus assuming that the field is always next to a freshwater body. If local circumstances are different, the dissolved pesticide is emitted to agricultural or natural soil next to the field, and should be reported as such for characterization. Moreover, the model's database includes some general scenarios for European climate and soil conditions, which can be different from site-specific conditions. This could lead to a difficulty in applying the model to different geographical areas, characterized by other soil and climate conditions, thus preventing from obtaining realistic results.

When using PestLCI 2.0 in LCA practice, it should be considered that: (1) the model calculates emissions to groundwater, for which characterization factors are absent in most frequently used LCIA methods; (2) neither PestLCI 2.0 nor LCIA methods consider that most pesticide removed from the field by wind drift during application, reported as emission to air in PestLCI 2.0, is in the form of droplets that are mainly deposited next to the field. For this reason, emissions due to wind drift could be reported and characterized as emissions to surface water or soil, depending on local circumstances, as it will be done in this work.

The goal of this study is to evaluate the results of the application of PestLCI 2.0 to maize production in the experimental farm of Vallevicchia, located near Caorle (province of Venice, Northern Italy) using site-specific soil and climate data, which were added for this purpose in PestLCI database. Moreover, the results obtained with the soil data of the Vallevicchia area were compared with those obtained assuming maize cultivation on other soils widespread in the

surrounding areas. The study was carried out within the LIFE project AGRICARE (Introducing innovative precision farming techniques in AGRiculture to decrease CARbon Emissions).

## **2. Materials and methods**

### **2.1 Update of PestLCI 2.0**

For this work, PestLCI model version 2.0.8 was used, which, in addition to removing errors in the implementation of model equations, introduces a new regression for volatilization from leaves (Dijkman 2014). The current regression relates the volatilization rate constant to the vapour pressure on basis of measurements of volatilization of pesticides from plant leaves (Guth et al., 2004). This regression was introduced (1) to remove the dependence of the volatilization rate constant on the pesticide application rate, and (2) because the volatilization rate was found to be overestimated for volatile pesticides (vapour pressure  $>10^{-3}$  Pa).

In addition, one new climate profile and eight soil profiles representative for the Vallevecchia area were introduced. Model inputs such as pesticide active ingredient, climate, soil, crop type and application month, as well as application and field characteristics, were set to reflect local circumstances. Default values were used for the other adjustable parameters.

### **2.2 Description of agronomic, climate and soil data**

Maize is cultivated with a conventional tillage technique in the studied area. Three main phases for the use of pesticides can be identified: 1) the pre-emergence phase, in which the pesticides are spread before seeding or before plants emerge from the soil; 2) post-emergence, which corresponds to the leaf development of the crop; 3) treatment for insects which corresponds to the inflorescence development. Pesticide 1 and 2 were used in both pre and post-emergence, whereas pesticide 3 was used only for the treatment of insects. The area of the field is 0.35 ha.

Climatological data have been obtained on the basis of data referred to period 1/1/1994-31/12/2014 which were acquired at the station of Lugugnana (Portogruaro) (ARPAV, 2016a). The climatological data used in this study come from station n° 166 (Lugugnana di Portogruaro, Venice Province).

Soil data have been collected from soil map of ARPAV (2016b). Every cartographic unit in the soil map is provided with a link to the list of the included Soil Typological Units (UTS). Each UTS, identified by both a name and an acronym, is described in detail, with the most relevant physical and chemical soil characteristics, the landscape unit and both the Soil Taxonomy and World Reference Base soils classifications.

The studied site insists on reclaimed lagoon areas derived from Piave, Livenza and Tagliamento rivers deposits. Soils described in this area and accounted for in the study (BIB1, CAB1, CFO1, CON1, CRL1, CTU1, QUA1 and TDF1) are

generally deep, with a typical Ap/Bg/Cg<sup>6</sup> or Ap/Cg horizons sequence and a moderate organic carbon content and alkaline reaction.

Soils differ in texture, which is silty clay loam (TDF1, CFO1, CTU1, CAB1) or silty loam (BIB1, QUA1, CON1, CRL1) and also for the presence of organic horizons (O) in some UTS (CTU1, CAB1) which lie, anyway, at a depth greater than 1 m, which was therefore not considered in the computation. These UTS are all suitable for maize cultivation but they have different characteristics and limitations which provide different attitudes to crop production.

### 3. Results and discussion

Table 1 shows, for each active ingredient and soil, the obtained fraction of emission to air, surface water or off-field soils (i.e. natural or agricultural fields located next to the field where the pesticide is applied), ground water and the fraction degraded or uptaken by plants or soil. Moreover, the minimum, maximum and average values, the standard deviation and the coefficient of variation have been included.

Firstly, it is very interesting to note that the fraction degraded or uptaken by plants or soils varies greatly on the basis of the pesticide. As regards pesticide 1, this fraction is 0.6- 0.7, therefore a significant fraction is emitted to air and/or water. On the contrary, the fraction of pesticide 2 and pesticide 3 degraded or uptaken is always higher than 0.9 and often reaches 0.99. Therefore, the fraction emitted to air and water is small or negligible. Moreover, the period of pesticide application seems not to affect the fraction degraded or emitted. In fact, the fraction of pesticide 1 emitted during the pre-emergence is very similar to the one emitted in post-emergence. The same occurs for pesticide 2. The influence of soil type generally appears very weak. The only exception is the pesticide 2 applied in pre-emergence, where the c.v. is 41.

Results highlight that both the emissions to air and surface water or off-field soils are scarcely affected or completely not affected by soil variation. In particular, airborne emissions are the sum of two contributions, i.e. pesticide volatilization from leaves and top soil and both values depend mainly on meteorological conditions, on pesticide chemical properties and both pH and organic carbon content of soil, which in our case is moderate for all the soils considered. Therefore, the role of soil is negligible in those cases. Pesticide 1 and pesticide 3 show virtually identical values for all soils. For pesticide 1, this is because the  $K_{oc}$  at the pH of the studied soils is very low, meaning that almost all is dissolved, so that the properties of the soil have little influence on the emissions. In contrast, for pesticide 3, volatilization from soil occurs with at a very low rate, meaning that emissions to air are dominated by volatilization from leaves.

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<sup>6</sup> Ap: organo-mineral horizon interested by tillage or other disturbance; Bg: accumulation horizon with saturation with water; Cg: horizon which is little affected by pedogenetic processes and has saturation with water (SSS, 2006).

For pesticide 2, a high differentiation among the soils is found in pre-emergence (c.v.= 63.6%). As regards pesticide 2 in post-emergence, the results are very similar (c.v.= 4.7%). For pesticide 2 the decrease in differentiation after emergence is explained by the fact that emissions to air due to volatilization from leaves are typically 2 orders of magnitude higher than emissions due to volatilization from soil. Before emergence, there are no leaves, so that the variation in emissions resulting from differences in soil properties is visible.

Surface water (or off- field soil) emissions seem to be even less affected by soil characteristics (c.v. is 0%, 0.3% and 0% for pesticide 1, 2 and 3, respectively) if compared to air emissions. More in detail, surface water (or off-soil field) emissions consist of two contributions: wind drift loss (i.e. pesticide's droplets which are transported by wind and deposited on water or soil) and runoff, where the former is always at least one order of magnitude higher than the latter. However, the value of wind drift loss is only correlated to the application technique and the field size. Therefore, the results of PestLCI show that these values are completely independent from soil type. On the contrary, runoff fraction is strictly correlated to the characteristic of soil but it has a minor contribution on the total fraction emitted to surface water (or off-field soils).

The reason for wind drift dominating the off-field surface emissions is twofold: the field size modelled is small, resulting in more drift (the larger the field, the more drifting pesticide is deposited inside the field), and the slope of the field is 0, so that water not readily starts running off.

In contrast, Table 1 shows that soil type affects remarkably the emissions to groundwater (c.v. is about 14%, 40% and 18% for pesticide 1, pesticide 2 and pesticide 3, respectively), although the characteristics of the eight soils analysed are quite similar. However, a clear relationship between soil characteristics and the fractions of pesticide reaching ground water could not be identified. Since the emissions to this environmental matrix are leaded by many parameters (related to the type of pesticide, the type of soil and the meteorological conditions), the behaviour of the pesticide has a high variability. Emissions to groundwater consist of emissions due to: 1) leaching through the soil matrix and 2) emissions through macropores. As regards leaching, Pest LCI models the soil as a column, through which water moves downwards, taking the pesticide with it. However, the pesticide moves slower than water, because it is absorbed by soil. The factor that determines how much slower the pesticide moves compared to water is calculated from the density of the soil and its organic content, which differs per soil horizon. As far as the soil density is concerned, for each horizon a specific density is calculated from the sand content and the fraction of organic carbon. In addition, the fraction of pesticide absorbed (and which is thus unavailable for degradation) differs per soil horizon and also depends on the organic carbon content of the soil. Finally, the rate at which water moves downward through soil depends, amongst others, on the sand content of soil. Regarding macropores, it is important to remember that the total pore volume is the volume of water and air in the soil and that soil pores are classified into immobile, slow mobile and fast mobile pores. The fast ones are considered macropores (with a diameter >8 mm). PestLCI splits pores into immobile and mobile pores on basis of the fractions of sand, silt, and clay. Next, the mobile pores are split into slow and fast pores on a 70/30 basis for all soil types.



<b>Pesticide 1 (pre emergence)</b>	<b>TDF1</b>	<b>CFO1</b>	<b>CTU1</b>	<b>CAB1</b>	<b>BIB1</b>	<b>QUA1</b>	<b>CON1</b>	<b>CRL1</b>	<b>MIN</b>	<b>MAX</b>	<b>Average</b>	<b>Stand. Dev.</b>	<b>C.V. %</b>
emission to air	9.3E-02	9.3E-02	9.3E-02	9.3E-02	9.3E-02	9.3E-02	9.3E-02	9.3E-02	9.3E-02	9.3E-02	9.3E-02	0.0E+00	0.0
emission to surface water or off-field soil	2.3E-03	2.3E-03	2.3E-03	2.3E-03	2.3E-03	2.3E-03	2.3E-03	2.3E-03	2.3E-03	2.3E-03	2.3E-03	0.0E+00	0.0
emission to ground water	2.5E-01	3.1E-01	2.6E-01	3.3E-01	2.3E-01	3.1E-01	2.6E-01	2.3E-01	2.3E-01	3.3E-01	2.7E-01	<b>3.9E-02</b>	<b>14.3</b>
degradation and uptake (fraction)	6.6E-01	5.9E-01	6.5E-01	5.7E-01	6.7E-01	5.9E-01	6.5E-01	6.7E-01	5.7E-01	6.7E-01	6.3E-01	<b>3.9E-02</b>	6.2
<b>Pesticide 1 (post emergence)</b>													
emission to air	1.2E-01	1.2E-01	1.2E-01	1.2E-01	1.2E-01	1.2E-01	1.2E-01	1.2E-01	1.2E-01	1.2E-01	1.2E-01	1.5E-17	0.0
emission to surface water or off-field soil	1.3E-03	1.3E-03	1.3E-03	1.3E-03	1.3E-03	1.3E-03	1.3E-03	1.3E-03	1.3E-03	1.3E-03	1.3E-03	5.8E-11	0.0
emission to ground water	1.7E-01	2.2E-01	1.8E-01	2.3E-01	1.6E-01	2.2E-01	1.8E-01	1.6E-01	1.6E-01	2.3E-01	1.9E-01	<b>2.7E-02</b>	<b>14.1</b>
degradation and uptake	7.1E-01	6.6E-01	7.0E-01	6.5E-01	7.2E-01	6.6E-01	7.0E-01	7.2E-01	6.5E-01	7.2E-01	6.9E-01	<b>2.7E-02</b>	3.9
<b>Pesticide 2 (pre emergence)</b>													
emission to air	7.7E-05	8.7E-05	2.7E-05	1.2E-04	8.7E-05	2.0E-04	2.9E-04	1.8E-04	2.7E-05	2.9E-04	1.3E-04	8.3E-05	<b>63.1</b>
emission to surface water or off-field soil	9.5E-03	9.5E-03	9.4E-03	9.5E-03	9.5E-03	9.6E-03	9.6E-03	9.6E-03	9.4E-03	9.6E-03	9.5E-03	5.1E-05	0.5
emission to ground water	2.6E-03	5.3E-03	2.3E-03	7.1E-03	2.5E-03	6.2E-03	4.6E-03	3.3E-03	2.3E-03	7.1E-03	4.2E-03	<b>1.8E-03</b>	<b>43.1</b>
degradation and uptake	9.9E-01	9.9E-01	9.9E-01	9.8E-01	9.9E-01	9.8E-01	9.9E-01	9.9E-01	9.8E-01	9.9E-01	9.9E-01	<b>1.9E-03</b>	0.2
<b>Pesticide 2 (post emergence)</b>													
emission to air	2.5E-03	2.5E-03	2.4E-03	2.5E-03	2.5E-03	2.6E-03	2.8E-03	2.6E-03	2.4E-03	2.8E-03	2.5E-03	1.2E-04	4.7
emission to surface water or off-field soil	2.0E-02	2.0E-02	2.0E-02	2.0E-02	2.0E-02	2.0E-02	2.0E-02	2.0E-02	2.0E-02	2.0E-02	2.0E-02	4.1E-05	0.2

<b>Pesticide 1 (pre emergence)</b>	<b>TDF1</b>	<b>CFO1</b>	<b>CTU1</b>	<b>CAB1</b>	<b>BIB1</b>	<b>QUA1</b>	<b>CON1</b>	<b>CRL1</b>	<b>MIN</b>	<b>MAX</b>	<b>Average</b>	<b>Stand. Dev.</b>	<b>C.V. %</b>
emission to ground water	2.0E-03	3.8E-03	1.7E-03	5.1E-03	1.9E-03	4.5E-03	3.4E-03	2.5E-03	1.7E-03	5.1E-03	3.1E-03	<b>1.3E-03</b>	<b>41.1</b>
degradation and uptake	9.8E-01	9.7E-01	9.8E-01	9.7E-01	9.8E-01	9.7E-01	9.7E-01	9.8E-01	9.7E-01	9.8E-01	9.7E-01	<b>1.3E-03</b>	0.1
<b>Pesticide 3</b>													
emission to air	4.1E-04	4.1E-04	4.1E-04	4.1E-04	4.1E-04	4.1E-04	4.1E-04	4.1E-04	4.1E-04	4.1E-04	4.1E-04	0.0E+00	0.0
emission to surface water or off-field soil	2.7E-04	2.7E-04	2.7E-04	2.7E-04	2.7E-04	2.7E-04	2.7E-04	2.7E-04	2.7E-04	2.7E-04	2.7E-04	1.3E-09	0.0
emission to ground water	5.2E-02	6.9E-02	5.5E-02	7.5E-02	4.8E-02	6.9E-02	5.6E-02	4.8E-02	4.8E-02	7.5E-02	5.9E-02	<b>1.0E-02</b>	<b>17.6</b>
degradation and uptake	9.5E-01	9.3E-01	9.4E-01	9.2E-01	9.5E-01	9.3E-01	9.4E-01	9.5E-01	9.2E-01	9.5E-01	9.4E-01	<b>1.0E-02</b>	1.1

Table 1: Results of the application of PestLCI model for each active ingredient and for each soil type. Figures indicate the fraction of pesticide emitted in each environmental matrix



The assessment of the amount of pesticide which reaches the ground water through macropores is based on a tipping bucket approach. When it rains, the pores are filled, starting with the immobile pores, then the slow mobile, and finally the fast mobile. As a consequence of this approach, sandy soils have more mobile pores and can therefore store more water, so macropore flow occurs less often (Hall, 1993).

The weight of soil matrix contribution and the weight of macropores contribution depend on the type of pesticide. In this study, the relevance of transportation through macropores and that of leaching through the soil matrix are different for the three pesticides. The fraction of pesticide 1 which reaches groundwater through soil leaching is about one order of magnitude higher than that from macropores. In the case of pesticide 2, the two fractions are more or less of the same order of magnitude. Finally, the fraction of pesticide 3 which reaches groundwater through macropores is four-five orders of magnitude lower than that coming from soil matrix.

In conclusion, the study shows that soil characteristics affect greatly the fraction of pesticide which reaches groundwater. In particular, during the 'pre emergence' phase, they influence also 'degradation fraction'. On the contrary, the effect on surface water (or off-field soils) appears very low. Generally, the effect on air fraction is negligible, although the fate of pesticide 2 during the 'pre emergence' phase is seriously affected by soil variations.

Finally, the study has allowed us to highlight some important features of PestLCI related to soil characteristics and to provide some further comments for improving the model. The assumption that the ratio between slow mobile macropores and fast mobile macropores is the same in all type of soil (0.7 and 0.3, respectively) is too basic and it does not reflect the reality. The scientific literature reports that macropores occur more in structured soils (clayey and silty soils) and less in destructured soils (sandy soil) (Hall, 1993). This assumption of PestLCI 2.0 modifies the speed of water in sandy soil and the role of macropores in the emission to groundwater.

The best solution would be to set the fraction of macropores to the soil type. Another important feature is that the model considers only the top 1 meter depth of soil. This assumption is based on two motivations. Firstly, 1 meter seems sufficiently deep to draw the line between the technosphere and the ecosphere. In such way PestLCI 2.0 assumes that the field below 1 meter is not manipulated by agricultural practice. Secondly, PestLCI assumes that pesticide degradation stops below 1 meter. This hypothesis implies that when a pesticide reaches 1 m of depth, it will at some point reach the ground water. Therefore, the exact depth of water table is not important. It is evident that if the groundwater table is at less than 1 m (i.e. costal or spring areas), this assumption is misleading. Our final observation is that PestLCI 2.0 considers organic horizons as mineral horizons. In the model, organic carbon is only used to calculate the fraction of pesticide absorbed and the density of the soil horizon.

This simplification could be another limitation in the case of soils with a high level of organic carbon, because in such horizons the organic carbon has an important role especially in the downward movement of water and substances. Likewise, PestLCI 2.0 does not take into account the presence of rock fragments (soil skeleton > 2 mm) in the calculation of emissions to surface and ground water. This might be considered for future model updates as well.

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Yara Italia che gentilmente ha contribuito all'organizzazione del Welcome Party

**Knowledge grows**

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